PERIODIC MULTILAYER FILM

We have a periodic layer structure with two layers in the period. Layer 1 has index of refraction n_1, relative permittivity $\varepsilon_1 = n_1^2$, and thickness d_1, whereas layer 2 has n_2, ε_2 and d_2. The period of the layer structure is then

$$d = d_1 + d_2. \tag{1}$$

The layers are oriented in the x-y plane, perpendicular to the z direction, and have unity relative magnetic permeability. In each layer harmonic electromagnetic waves with frequency f travel up and down in the z direction. Let us define

$$\begin{aligned} k_0 &= 2\pi f/c = \omega/c, \qquad (2)\\ k_1 &= n_1 k_0 \;\text{ and }\; k_2 = n_2 k_0, \qquad (3) \end{aligned}$$

where ω is the angular frequency, c is the speed of light in vacuum, and k_i, $i = 0, 1, 2$ are the the angular repetencies in vacuum, layer 1 and layer 2, respectively. Let the E and D fields point in the x direction, so that the B and H fields point in the y direction. We then have the following expression for the E field in layer 1:

$$E(z) = E^+ \exp(ik_1 z) + E^- \exp(-ik_1 z), \tag{4}$$

and a corresponding expression for layer 2.

Eq. (2) yields the following expressions for the E field and the derivative of E with respect to z,

$$\begin{aligned} E(z) &= E(0)\cos(k_1 z) + (E'(0)/k_1)\sin(k_1 z), \qquad (5)\\ E'(z) &= -k_1 E(0)\sin(k_1 z) + E'(0)\cos(k_1 z). \qquad (6) \end{aligned}$$

If we have different materials in the two layers, there is a discontinuity in the index of refraction and permittivity when we go in the z direction from one material into the other material. Maxwell's equations then imply that E, B, and H are alle continuous across the layer interfaces. D is equal to the permittivity times E, so D must be discontinuos across the interface. Furthermore, Maxwell's equations imply that $E' = dE/dz$ is proportional to B, and hence continuous, whereas $H' = dH/dz$ is proportional to D and hence discontinuous across the interface.

Let us introduce three coloumn vectors

$$\mathbf{E}_0 = \begin{bmatrix} E(0) \\ E'(0) \end{bmatrix}, \quad \mathbf{E}_1 = \begin{bmatrix} E(d_1) \\ E'(d_1) \end{bmatrix}, \quad \mathbf{E}_2 = \begin{bmatrix} E(d_1+d_2) \\ E'(d_1+d_2) \end{bmatrix} \tag{7}$$

and two matrices

$$\mathbf{M}_1 = \begin{bmatrix} c_1 & s_1/k_1 \\ -s_1 k_1 & c_1 \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} c_2 & s_2/k_2 \\ -s_2 k_2 & c_2 \end{bmatrix}, \tag{8}$$

with

$$\begin{aligned} c_p &= \cos(k_p d_p) \;\text{ and} \qquad (9)\\ s_p &= \sin(k_p d_p) \quad \text{for } p \text{ equals 1 or 2.} \qquad (10) \end{aligned}$$

Then the continuity reqirements for the fields yield the following matrix equations

$$\mathbf{E}_2 = \mathbf{M}_2\mathbf{E}_1 = \mathbf{M}_2\mathbf{M}_1\mathbf{E}_0. \tag{11}$$

Then we have obtained what is called a transfer matrix formulation. It is very transparent and easily generalized to the case of more than two layers per period in the structure.

We seek solutions of the socalled Bloch wave form, where

$$E(z) = \exp(ikz)\ u(z), \tag{12}$$

where k is the angular repetency of the wave, and $u(z)$ is periodic with period d. For such solutions we get

$$\exp(ikd)\,\mathbf{E}_0 = \mathbf{E}_2 = \mathbf{M}_2\mathbf{E}_1 = \mathbf{M}_2\mathbf{M}_1\mathbf{E}_0. \tag{13}$$

The above equation is an eigenvalue equation for the matrix $\mathbf{M}_2\mathbf{M}_1$, where the eigenvalue of the matrix is

$$e = \exp(ikd) = \exp\left[ik\left(d_1 + d_2\right)\right]. \tag{14}$$

Problem 1)

Show that the eigenvalue equation (13) implies that e satisfies the equation

$$e^2 - e\left[2\cos(k_1d_1 + k_2d_2) - ((k_1 - k_2)^2/(k_1k_2))s_1s_2\right] + 1 = 0, \tag{15}$$

further implying that

$$\cos(kd) = \cos(k_1d_1 + k_2d_2) - \frac{(k_1 - k_2)^2}{2k_1k_2}\sin(k_1d_1)\sin(k_2d_2). \tag{16}$$

Equation (16) is a relationship between ω and k, and hence called a *dispersion equation.* This equation permits us to define three central properties of photonic crystals, namely *band, band gap and band edge.*

1. Band: A continuous frequency interval where the dispersion equation (16) has real solutions for k, *i.e.*, where the absolute value of the right-hand side is less than 1.
2. Band gap: A continuous frequency interval where the dispersion equation (16) has no real solutions for k, *i.e.*, where the absolute value of the right-hand side is greater than 1.
3. Band edge: The beginning or the end of a band, *i.e.*, where the absolute value of the right-hand side of (16) is equal to 1.

Problem 2)

Let us assume that we have a nonzero refractive index contrast, *i.e.*. that d_1 and d_2 are both nonzero, and $n_1 \neq n_2$. Show that the dispersion equation (16) implies that we have a band gap if

$$k_1d_1 + k_2d_2 = N\pi, \tag{17}$$

where N is a nonzero integer.

Problem 3)

As shown in Problem (2), we have a band gap if the angular frequency is equal to an integer multiple of

$$\omega_0 = \frac{\pi c}{n_1 d_1 + n_2 d_2}. \tag{18}$$

Let us note that in Eq. (16), $\cos(k_1 d_1 + k_2 d_2)$ is equal to $(-1)^N$ for $\omega = N\omega_0$. Let us then consider the case of a small refractive-index difference n_Δ between the layers:

$$|n_\Delta| = |n_1 - n_2| << n_1. \tag{19}$$

We note with a small refractive index difference, the absolute value of the last term on the right hand side of (16) is much smaller than 1. Consequently, we need only a small deviation

$$\omega_\Delta = \omega - N\omega_0. \tag{20}$$

in the angular frequency to make the right-hand side of (16) equal to $(-1)^N$

Do a second-order power series expansion of the right-hand side as a function of ω_Δ/ω_0, and obtain an analytic approximation for the distance ω_Δ between the band edge and the band gap center $N\omega_0$.

Hint: In the series expansion of the right-hand side with respect to ω_Δ we get a first-order term from the product of the sines:

$$s_N = \partial_\omega \left(\sin\left(\omega n_1 d_1/c\right) \sin\left(\omega n_2 d_2/c\right)\right), \tag{21}$$

with the partial derivative evaluated at $\omega = N\omega_0$.

Problem 4)

Let us consider the case when ω is an integer multiple N of ω_0, and let us again consider the case of a small refractive-index difference n_Δ between the layers. Then we have the following expression for k

$$k = N\pi/d + k_\Delta, \tag{22}$$

where N is an integer and k_Δ is small compared to π/d.

Do a second-order series expansions of the left-hand side of Eq. (16), and find an analytic approximations for k_Δ .

Problem 5)

Let us consider the case of small frequency,

$$k_1 d_1 + k_2 d_2 << 1, \tag{23}$$

and let us define what is called the effective index the Bloch wave in the layer structure,

$$n = ck/\omega. \tag{24}$$

Show that Eq. (16) for small frequencies implies that the square of the effective index can be expressed as the mean value of the square of the refractive index in the layer structure:

$$n^2 = \left(\frac{ck}{\omega}\right)^2 = \frac{n_1^2 d_1 + n_2^2 d_2}{d_1 + d_2}. \tag{25}$$

Problem 6)

The transfer matrix formalism expressed in Equation (11) is a recursive formula where the E field and its z derivative on top of layer 2 are expressed as a layer-2 matrix times the E field and its z derivative on top of layer 1, which in turn are expressed as a layer-1 matrix times the E field and its z derivative on top of layer 0. Equation (11) can be generalized to

$$\mathbf{E}_p = \mathbf{M}_p \mathbf{E}_{p-1}. \tag{26}$$

For numerical stability we prefer to have a recursion relationship for $Z_p = E'_p/E_p$ instead of E_p og E'_p . Find a recursive formula where Z_p can be computed from Z_{p-1}.

Problem 7) (Coding)

Use Eq. (16) to find the angular frequency ω as a function of k for the lowest 3 bands of the first Brillouin zone, *i.e.*, for $-\pi/d < k < \pi/d$. Let $n_1 = 1$, $n_2 = 1,5$ and $d_1 = d_2$. Make plots of ω versus k . Also make plots of ω versus k with k spanning 3 Brillouin zones *i.e.*, for $-3\pi/d < k < 3\pi/d$. In the last plot, include only the solutions of (16) that are close to the straight line given by the equation

$$(\omega/c)\,(n_1 d_1 + n_2 d_2) = k_1 d_1 + k_2 d_2 = k(d_1 + d_2). \tag{27}$$

Updated 5 september, 2019.